

Interface roughness and polar optical phonon scattering in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTDs

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Abstract. The contributions of interface roughness scattering and polar optical phonon scattering to the valley current of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ resonant tunnelling diodes (RTDs) are theoretically found to be comparable. An $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTD design is suggested to experimentally observe the phonon peak which has never been observed in this material system. Such a device will provide a calibration point for the theoretical calculations.

For most resonant tunnelling diodes (RTDs), sp^3s^* calculations indicate that the valley current at room temperature is largely the result of coherent transport through the second resonant state in the well [1, 2]. State-of-the-art RTDs use an InAs notch in the well to increase the separation of the first and second resonant states [3]. We are aware of only one theoretical investigation of incoherent scattering in these devices [4]; interface roughness was found to contribute far more to the valley current than polar optical phonon scattering. We find the relative contributions to be comparable. An $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTD design is presented to observe the phonon peak [5–7] which has never been observed in this material system. Such a device will provide a calibration point for the theory.

Our calculations use a single-band tight-binding model and the scattering is included with the models and self-energies described in appendix A of [8]. Interface roughness is modelled with 5 nm exponential correlation [8, 9]. The bulk $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ polar optical phonon model is used. Self-energies are included using the multiple sequential scattering algorithm illustrated by figure 4 of [8] with $N = 4$. The electrostatic potential is calculated self-consistently in the absence of incoherent scattering and it is then used for the scattering calculations [9].

We are not aware of any studies of the confined and interface phonon modes in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTDs, while numerous studies exist for the GaAs/AlAs devices [7, 10]. For a GaAs/AlAs RTD with 2.5 nm AlAs barriers and a 5 nm GaAs well, the phonon peak resulting from bulk phonons and the phonon peak resulting from confined and interface modes are essentially identical [11]. Therefore, the bulk phonon model should provide an accurate prediction of the shape, magnitude and voltage position of the phonon peak.

Figure 1 shows both the experimental and calculated current–voltage (I – V) curves for an $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$

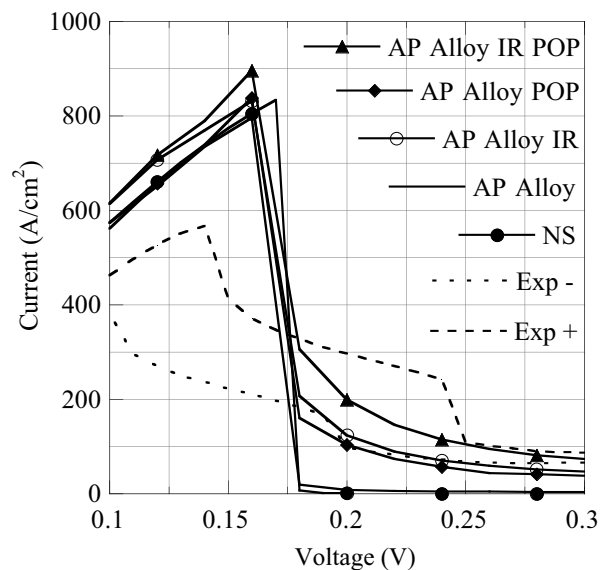


Figure 1. Comparison of experimental and calculated I – V s at 300 K including various incoherent scattering mechanisms. The RTD consists of $10^{18} \text{ cm}^{-3} \text{ n}^+$ $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ leads, 2 nm intrinsic $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ spacer layers, 2.9 nm AlAs barriers, and a 1.5 nm/2.0 nm/1.5 nm $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InAs}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ well.

InAs RTD at room temperature. Interface roughness is included at all interfaces. The experimental I – V is asymmetric, although the structure is nominally symmetric. We have flipped the third quadrant onto the first to show the asymmetry. The simulation with the lowest valley current is the coherent tunnelling calculation labelled ‘NS’. The inclusion of acoustic phonon and alloy scattering raises the valley current, but it is barely noticeable on a linear scale. The curve labelled ‘AP Alloy IR’ includes scattering from acoustic phonons, alloy disorder and interface roughness.

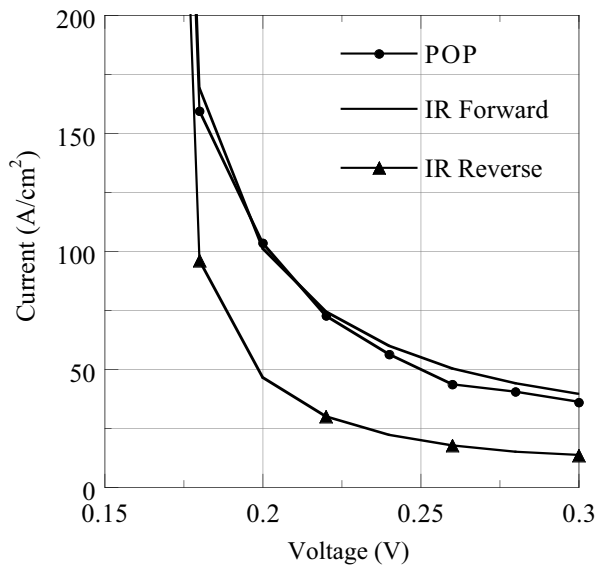


Figure 2. I - V characteristic of the same device as in figure 1 but with interface roughness on alternate interfaces.

The curve labelled 'AP Alloy POP' includes scattering from acoustic phonons, alloy disorder and polar optical phonons. These calculations indicate that the contribution from interface roughness scattering and polar optical scattering are comparable. The curve labelled 'AP Alloy IR POP' includes scattering from all four scattering mechanisms.

In figure 2 we investigate the effects of asymmetric roughness [9]. The curve labelled 'POP' is replotted from figure 1 where it is labelled 'AP Alloy POP'. For the curve labelled 'IR Forward', the first, third and fifth interfaces counting from the emitter are rough and the other interfaces are smooth. For the curve labelled 'IR Reverse', the rough and smooth interfaces are interchanged. For the 'IR Reverse' curve, the excess current is scattered from the rough InAs interface in the well since scattering from the second and sixth interfaces is negligible [9]. A comparison of the 'IR Reverse' and 'IR Forward' curves indicates that the scattering from the first AlAs interface is roughly twice as large as the scattering from the InAs interface. Knowing the relative contributions from the InAs and AlAs interfaces and taking into account the difference in material parameters, we can assert that our result for the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTD is consistent with our result for a GaAs/AlAs RTD [9].

A device that displayed the phonon peak would be useful for assessing the theory. The calculated I - V of such a device at 4.2 K is shown in figure 3. The three curves show the coherent tunnelling calculation labelled 'NS', the calculation including acoustic phonons, alloy disorder and interface roughness labelled 'AP Alloy IR', and the calculation including acoustic phonons, alloy disorder and polar optical phonons labelled 'AP Alloy POP'. We note that (i) the reduction of the peak current in the presence of interface roughness scattering is a numerical artefact of the finite truncation of the scattering series and the lack of full charge self-consistency, and (ii) these approximations have little impact on the calculation of the valley current which

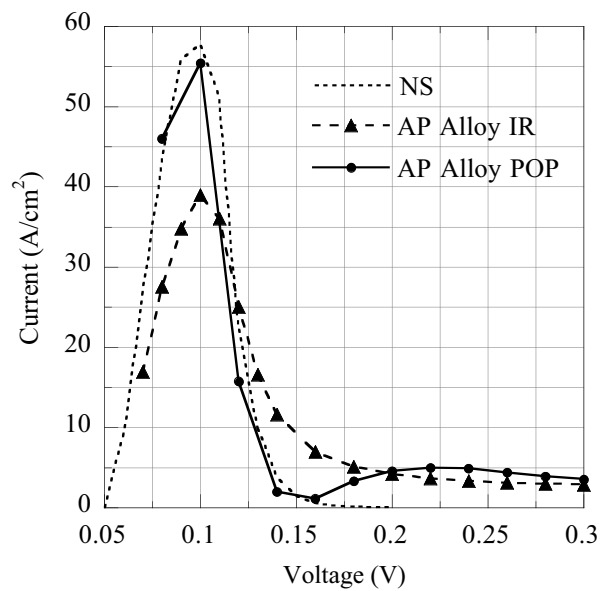


Figure 3. I - V characteristic at 4.2 K which exhibits a phonon peak. The RTD has $10^{18} \text{ cm}^{-3} \text{ n}^+ \text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ leads, 50 nm intrinsic $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ spacer layers, a 2.9 nm AlAs emitter barrier, a 2 nm/2 nm/2 nm $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InAs}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ well and a 2.3 nm collector barrier.

is our concern [8, 12]. The phonon peak should be clearly visible in such a structure.

In summary we find the relative contributions of interface roughness scattering and polar optical phonon scattering to the valley current of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTDs to be comparable, which is consistent with results for a GaAs/AlAs RTD [9]. For the GaAs/AlAs RTD, the phonon peak is clearly visible. Figure 3 shows that the phonon peak should be observable for $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{AlAs}/\text{InAs}$ RTDs as well. Experimental data [5–7] are required to assess the theory.

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